10-701 Introduction to Machine Learning (PhD)
Lecture 14: Learning Theory

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Slides based on Tom Mitchell's 10701 Fall 2016 material
Readings: [TM] chapter 7
Nina Balcan's notes on generalization guarantees: http://www.cs.cmu.edu/~ninamf/courses/601sp15/sc-2015.pdf

Announcements

- Project report due Friday
  - Follow the requirements!
- Monday 3/18 and Wednesday 3/20:
  - Class starts at 11!
  - We will do a midterm review

Computational Learning Theory

- What general laws constrain inductive learning?
- Want theory to relate
  – Number of training examples
  – Complexity of hypothesis space
  – Accuracy to which target function is approximated
  – Manner in which training examples are presented
  – Probability of successful learning

* See annual Conference on Computational Learning Theory

Sample Complexity

How many training examples suffice to learn target concept

1. If learner proposes instances as queries to teacher?
   - learner proposes x, teacher provides f(x)
2. If teacher (who knows f(x)) generates training examples?
   - teacher proposes sequence $\{(x^1, f(x^1)), \ldots (x^n, f(x^n))\}$
3. If some random process (e.g., nature) generates instances, and teacher labels them?
   - instances drawn according to $P(X)$

Sample Complexity 3

Problem setting:

- Set of instances X
- Set of hypotheses $H = \{h : X \to \{0, 1\}\}$
- Set of possible target functions $C = \{c : X \to \{0, 1\}\}$
- Sequence of training instances drawn at random from $P(X)$ teacher provides noise-free label $c(x)$

Learner outputs a hypothesis $h \in H$ such that

$$h = \arg\min_{h \in H} \ error_{train}(h)$$

Example: Learning decision trees

Take $X = (X_1, \dots, X_n) \quad s.t. X_i \in \{0,1\}$

$Y_i \in \{0,1\}$

Let H be the set of decision trees:

$H = \{h : X \to Y\}$

How many possible values of X?

How many possible trees?

How many training examples needed to find the right tree?

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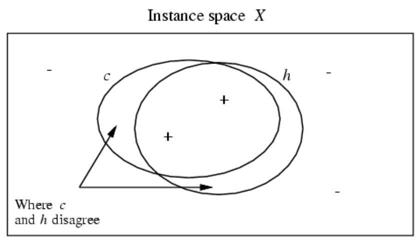
Generalizing beyond training is impossible unless we add assumptions

training examples are provided according to distribution P(X)

True Error of a Hypothesis



The *true error* of h is the probability that it will misclassify an example drawn at random from $P(X)$

$$error_{true}(h) \equiv \Pr_{x \sim P(X)}[h(x) \neq c(x)]$$

Two notions of error

Training error of hypothesis h with respect to target concept c

- How often $h(x) \neq c(x)$ over training instances D

$$error_{train}(h) \equiv \Pr_{x \in D}[h(x) \neq c(x)] = \frac{1}{|D|} \sum_{x \in D} \delta(h(x) \neq c(x))$$

training examples D

True error of hypothesis h with respect to c

- How often $h(x) \neq c(x)$ over future instances drawn at random from $\mathcal{D}$

$$error_{true}(h) \equiv \Pr_{x \sim P(X)}[h(x) \neq c(x)]$$

Probability distribution P(X)

Overfitting

Consider a hypothesis h and its

- Error rate over training data: $error_{train}(h)$
- True error rate over all data: $error_{true}(h)$

We say h overfits the training data if

$$error_{true}(h) > error_{train}(h)$$

Amount of overfitting =

$$error_{true}(h) - error_{train}(h)$$

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Amount of overfitting =

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Can we bound $error_{true}(h)$ in terms of $error_{train}(h)$??

$$error_{train}(h) \equiv \Pr_{x \in D}[h(x) \neq c(x)] = \frac{1}{|D|} \sum_{x \in D} \delta(h(x) \neq c(x))$$

training examples

$$error_{true}(h) \equiv \Pr_{x \sim P(X)}[h(x) \neq c(x)]$$

Probability distribution P(x)

if D was a set of examples drawn from $P(X)$ and ***independent*** of h, then we could use standard statistical confidence intervals to determine that with 95% probability, $error_{true}(h)$ lies in the interval:

$$error_D(h) \pm 1.96 \sqrt{\frac{error_D(h)\,(1 - error_D(h))}{n}}$$

but D is the ***training data*** for h ….

Version Spaces

$c : X \rightarrow \{0,1\}$

A hypothesis h is **consistent** with a set of training examples D of target concept c if and only if $h(x) = c(x)$ for each training example $\langle x, c(x) \rangle$ in D.

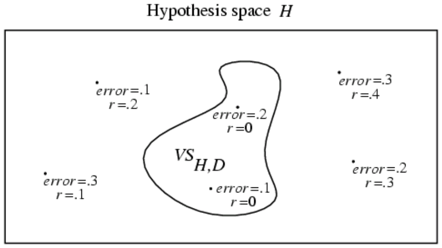
$$Consistent(h, D) \equiv (\forall \langle x, c(x) \rangle \in D)\; h(x) = c(x)$$

The **version space**, $VS_{H,D}$, with respect to hypothesis space H and training examples D, is the subset of hypotheses from H consistent with all training examples in D.

$$VS_{H,D} \equiv \{h \in H | Consistent(h, D)\}$$

Exhausting the version space

Hypothesis space H



(r = training error, $error$ = true error)

Definition: The version space $VS_{H,D}$ with respect to training data D is said to be ϵ-**exhausted** if every hypothesis h in $VS_{H,D}$ has true error less than ϵ.

$$(\forall h \in VS_{H,D})\; error_{true}(h) < \epsilon$$

How many examples will ε-exhaust the version space?

Theorem: [Haussler, 1988].

If the hypothesis space H is finite, and D is a sequence of $m \geq 1$ independent random examples of some target concept c, then for any $0 \leq \epsilon \leq 1$, the probability that the version space with respect to H and D is not ϵ-exhausted (with respect to c) is less than

$$|H| e^{-\epsilon m}$$

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Interesting! This bounds the probability that any consistent learner will output a hypothesis h with $error(h) \geq \epsilon$

Any(!) learner that outputs a hypothesis consistent with all training examples (i.e., an h contained in VSH,D)

What it means

[Haussler, 1988]: probability that the version space is not ε-exhausted after *m* training examples is at most $|H|e^{-\epsilon m}$

$$\Pr[(\exists h \in H) s.t. (error_{train}(h) = 0) \wedge (error_{true}(h) > \epsilon)] \leq |H|e^{-\epsilon m}$$

Suppose we want this probability to be at most δ

1. How many training examples suffice?

$$m \geq \frac{1}{\epsilon}(\ln|H| + \ln(1/\delta))$$

2. If. $error_{train}(h) = 0$ then with probability at least (1-δ):

$$error_{true}(h) \leq \frac{1}{m}(\ln|H| + \ln(1/\delta))$$

Example: H is Conjunction of up to N Boolean Literals

$$m \geq \frac{1}{\epsilon}(\ln|H| + \ln(1/\delta))$$

Consider classification problem f:X→Y:

- instances: $X = (X_1, X_2, X_3, X_4)$ where each X_i is boolean
- Each hypothesis in H is a rule of the form:
  - IF $(X_1, X_2, X_3, X_4) = (0,?,1,?)$, THEN Y=1, ELSE Y=0
  - i.e., rules constrain any subset of the X_i

How many training examples *m* suffice to assure that with probability at least 0.99, *any* consistent learner using H will output a hypothesis with true error at most 0.05?

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How many training examples *m* suffice to assure that with probability at least 0.99, *any* consistent learner using H will output a hypothesis with true error at most 0.05?

$$|H| = 3^4$$

$$m \geq \frac{1}{0.05}\left(\ln(|H|) + \ln(\frac{1}{0.01})\right)$$

Example: Depth 2 Decision Trees

$$m \geq \frac{1}{\epsilon}(\ln|H| + \ln(1/\delta))$$

Consider classification problem f:X→Y:

- instances: $X = <X_1 \ldots X_N>$ where each X_i is boolean
- learned hypotheses are decision trees of depth 2, using only two variables

How many training examples *m* suffice to assure that with probability at least 0.99, *any* learner that outputs a consistent depth 2 decision tree will have true error at most 0.05?

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Consider classification problem f:X→Y:

- instances: $X = <X_1 \ldots X_N>$ where each X_i is boolean
- learned hypotheses are decision trees of depth 2, using only two variables

$\binom{N}{2}$ **Trees** $= \frac{N!}{(N-2)!2!} = \frac{N(N-1)}{2}$ 2^4 **ways to label the nodes**

$$|H| = 8N(N-1)$$

How many training examples *m* suffice to assure that with probability at least 0.99, *any* learner that outputs a consistent depth 2 decision tree will have true error at most 0.05?

$$m \geq \frac{1}{0.05}\left(\ln(8N(N-1)) + \ln(\frac{1}{0.01})\right)$$

PAC learning

Consider a class C of possible target concepts defined over a set of instances X of length n, and a learner L using hypothesis space H.

Definition: C is **PAC-learnable** by L using H if for all $c \in C$, distributions $\mathcal{D}$ over X, ϵ such that $0 < \epsilon < 1/2$, and δ such that $0 < \delta < 1/2$, learner L will with probability at least $(1-\delta)$ output a hypothesis $h \in H$ such that $error_{\mathcal{D}}(h) \leq \epsilon$, in time that is polynomial in $1/\epsilon$, $1/\delta$, n and $size(c)$.

PAC learning

Consider a class C of possible target concepts defined over a set of instances X of length n, and a learner L using hypothesis space H.

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Sufficient condition:

Holds if learner L requires only a polynomial number of training examples, and processing per example is polynomial

Agnostic learning

So far, assumed $c \in H$

Agnostic learning setting: don't assume $c \in H$

- What do we want then?
  - The hypothesis h that makes fewest errors on training data
- What is sample complexity in this case?

$$m \geq \frac{1}{2\epsilon^2}(\ln|H| + \ln(1/\delta))$$

Here ε is the difference between the training error and true error of the output hypothesis (the one with lowest training error)

Additive Hoeffding Bounds – Agnostic Learning

- Given m independent flips of a coin with true Pr(heads) = θ we can bound the error ϵ in the maximum likelihood estimate $\hat{\theta}$

$$\Pr[\theta > \hat{\theta} + \epsilon] \leq e^{-2m\epsilon^2}$$

- Relevance to agnostic learning: for any ***single*** hypothesis *h*

$$\Pr[error_{true}(h) > error_{train}(h) + \epsilon] \leq e^{-2m\epsilon^2}$$

- But we must consider all hypotheses in H

$$\Pr[(\exists h \in H) error_{true}(h) > error_{train}(h) + \epsilon] \leq |H| e^{-2m\epsilon^2}$$

- So, with probability at least (1-δ) every h satisfies

$$error_{true}(h) \leq error_{train}(h) + \sqrt{\frac{\ln|H| + \ln\frac{1}{\delta}}{2m}}$$

General Hoeffding Bounds

- When estimating parameter θ inside [a,b] from *m* examples

$$P(|\hat{\theta} - E[\hat{\theta}]| > \epsilon) \leq 2e^{\frac{-2m\epsilon^2}{(b-a)^2}}$$

- When estimating a probability θ is inside [0,1], so

$$P(|\hat{\theta} - E[\hat{\theta}]| > \epsilon) \leq 2e^{-2m\epsilon^2}$$

- And if we're interested in only one-sided error, then

$$P((E[\hat{\theta}] - \hat{\theta}) > \epsilon) \leq e^{-2m\epsilon^2}$$

$$m \geq \frac{1}{2\epsilon^2}(\ln|H| + \ln(1/\delta))$$

Here ε is the difference between the training error and true error of the output hypothesis (this holds for all h in H)

But, the output h with lowest training error might not give us the h* with lowest true error. How far can true error of h be from h* ?

$$m \geq \frac{1}{2\epsilon^2}(\ln|H| + \ln(1/\delta))$$

Here ε is the difference between the training error and true error of the output hypothesis (this holds for all h in H)

But, the output h with lowest training error might not give us the h* with lowest true error. How far can true error of h be from h* ?

$$error_{true}(h) \leq error_{true}(h^*) + 2\epsilon$$

best training error hypothesis

best true error hypothesis

$$m \geq \frac{1}{\epsilon}(\ln|H| + \ln(1/\delta))$$

Question: If H = {h | h: X →Y} is infinite, what measure of complexity should we use in place of |H| ?

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Answer: The largest subset of X for which H can guarantee zero training error (regardless of how it is labeled)

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VC dimension of H is the size of this subset

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Informal intuition:

- decision tree example: how many labels do we need to see to learn h?

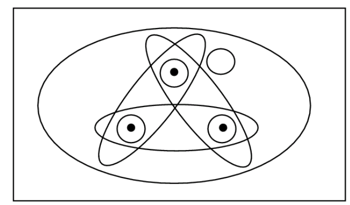
Shattering a set of instances

a labeling of each member of S as positive or negative

Definition: a **dichotomy** of a set S is a partition of S into two disjoint subsets.

Definition: a set of instances S is **shattered** by hypothesis space H if and only if for every dichotomy of S there exists some hypothesis in H consistent with this dichotomy.

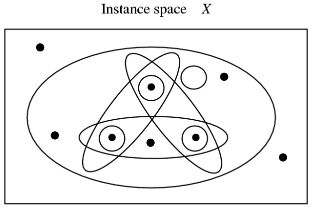
Instance space X



The Vapnik-Chervonenkis Dimension

Definition: The **Vapnik-Chervonenkis dimension**, $VC(H)$, of hypothesis space H defined over instance space X is the size of the largest finite subset of X shattered by H. If arbitrarily large finite sets of X can be shattered by H, then $VC(H) \equiv \infty$.

Instance space X



VC(H)=3

Sample Complexity based on VC dimension

How many randomly drawn examples suffice to ε-exhaust $VS_{H,D}$ with probability at least (1-δ)?

ie., to guarantee that any hypothesis that perfectly fits the training data is probably (1-δ) approximately (ε) correct

$$m \geq \frac{1}{\epsilon}(4\log_2(2/\delta) + 8VC(H)\log_2(13/\epsilon))$$

Compare to our earlier results based on |*H*|:

$$m \geq \frac{1}{\epsilon}(\ln(1/\delta) + \ln|H|)$$

VC dimension: examples

Consider X = <, want to learn c:X→{0,1}

What is VC dimension of

- Open intervals:

  H1: if $x > a$ then $y = 1$ else $y = 0$

  H2: if $x > a$ then $y = 1$ else $y = 0$
  or, if $x > a$ then $y = 0$ else $y = 1$

- Closed intervals:

  H3: if $a < x < b$ then $y = 1$ else $y = 0$

  H4: if $a < x < b$ then $y = 1$ else $y = 0$
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VC dimension: examples

Consider X = <, want to learn c:X→{0,1}

What is VC dimension of

- Open intervals:

  H1: if $x > a$ then $y = 1$ else $y = 0$ VC(H1)=1

  H2: if $x > a$ then $y = 1$ else $y = 0$ VC(H2)=2
  or, if $x > a$ then $y = 0$ else $y = 1$

- Closed intervals:

  H3: if $a < x < b$ then $y = 1$ else $y = 0$ VC(H3)=2

  H4: if $a < x < b$ then $y = 1$ else $y = 0$ VC(H4)=3
  or, if $a < x < b$ then $y = 0$ else $y = 1$

VC dimension: examples

What is VC dimension of lines in a plane?

- $H_2 = \{ ((w_0 + w_1 x_1 + w_2 x_2) > 0 \rightarrow \quad y=1) \}$

VC dimension: examples

What is VC dimension of

- $H_2 = \{ ((w_0 + w_1 x_1 + w_2 x_2) > 0 \rightarrow \quad y=1) \}$
  $VC(H_2)=3$

- For H_n = linear separating hyperplanes in n dimensions, $VC(H_n)=n+1$

For any finite hypothesis space H, can you give an upper bound on VC(H) in terms of |H| ?
(hint: yes)

More VC Dimension Examples to Think About

- Logistic regression over n continuous features
  - Over n boolean features?
- Decision trees defined over n boolean features

  F: <X_1, ... X_n> → Y
- Decision trees of depth 2 defined over n features
- Naïve Bayes defined over n boolean features
- How about 1-nearest neighbor?

Tightness of Bounds on Sample Complexity

How many examples m suffice to assure that any hypothesis that fits the training data perfectly is probably (1-δ) approximately (ε) correct?

$$m \geq \frac{1}{\epsilon}(4\log_2(2/\delta) + 8VC(H)\log_2(13/\epsilon))$$

How tight is this bound?

Shatter coefficient H[m]

for $S \subseteq X$, where $S = \{x_1 \dots x_m\}$, define $H(S)$ as the set of distinct labelings of S induced by H

$$H(S) \equiv \{\langle h(x_1) \dots, h(x_m)\rangle \mid h \in H)\}$$

and define $H[m]$ as the maximum number of ways to label m instances of X

$$H[m] \equiv \max_{S \subseteq X, |S|=m} |H(S)|$$

If H can shatter a subset of size m, then $H[m] =$

Note $VCdim(H) \equiv$ largest m for which $H[m] = 2^m$

Shatter coefficient H[m]

Sauer's Lemma: Let $VCdim(H) = d$. Then

1. for all m, $H[m] \leq \Phi_d(m)$, where $\Phi_d(m) \equiv \sum_{i=0}^{d} \binom{m}{i}$
2. for $m > d$,

$$\Phi_d(m) \leq (1+m)^d$$
$$\Phi_d(m) \leq \left(\frac{em}{d}\right)^d$$

Sample Complexity - Summary

How many randomly drawn examples suffice to ε-exhaust $VS_{H,D}$ with probability at least (1-δ)?

ie., to guarantee that any hypothesis that perfectly fits the training data is probably (1-δ) approximately (ε) correct

$$m \geq \frac{1}{\epsilon}(\ln(1/\delta) + \ln|H|)$$ |H|

$$m \geq \frac{1}{\epsilon}(4\log_2(2/\delta) + 8VC(H)\log_2(13/\epsilon))$$ VC(H)

$$m > \frac{2}{\epsilon}(\log_2(1/\delta) + \log_2(3\ H[2m]))$$ H[m]

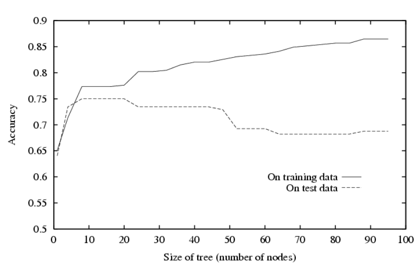
* also Rademacher complexity

Agnostic Learning: VC Bounds

[Schölkopf and Smola, 2002]

With probability at least (1-δ) every $h \in H$ satisfies

$$error_{true}(h) < error_{train}(h) + \sqrt{\frac{VC(H)(\ln\frac{2m}{VC(H)}+1)+\ln\frac{4}{\delta}}{m}}$$



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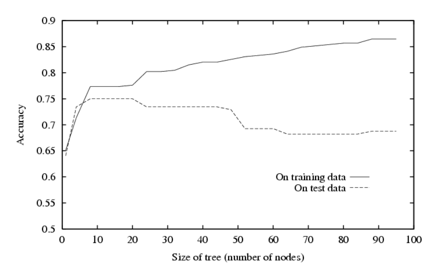

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$$m > \frac{2}{\epsilon}(\log_2(1/\delta) + \log_2(3\ H[2m]))$$ H[m]

* also Rademacher complexity

With probability $\geq (1-\delta)$, $(error_{true} - error_{train}) \leq \epsilon$

(1) for all $h \in H$ such that $error_{train} = 0$,

$$\epsilon = \frac{\ln|H| + \ln(1/\delta)}{m}$$ finite H

(2) for all $h \in H$

Agnostic

$$\epsilon = \sqrt{\frac{\ln|H| + \ln(1/\delta)}{2m}}$$ finite H

(3) for all $h \in H$

Agnostic

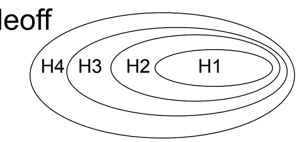
$$\epsilon = 8\sqrt{\frac{VC(H)(\ln\frac{m}{VC(H)} + 1) + \ln(8/\delta)}{2m}}$$ infinite H

We stopped here in lecture 14

Structural Risk Minimization

[Vapnik]

Which hypothesis space should we choose?
- Bias / variance tradeoff



SRM: choose H to minimize bound on expected true error!

$$error_{true}(h) < error_{train}(h) + \sqrt{\frac{VC(H)(\ln\frac{2m}{VC(H)} + 1) + \ln\frac{4}{\delta}}{m}}$$

* unfortunately a somewhat loose bound...

Rademacher Complexity

Key idea: complexity of H is its ability to fit noise labels.

Advantages:

- applies to real-valued functions (e.g., regression)
- is sensitive to P(X), and particular training set
- gives tighter bounds than VC dimension
- widely used in modern learning theory

Rademacher Complexity Setting

Learn $f : X \to Y$, where $Y \in \{-1, +1\}$

Note:
if $h(x) = y$, then $yh(x) = 1$
if $h(x) \neq y$, then $yh(x) = -1$

so error of h on sample $S = \{\langle x_1, y_1 \rangle, \ldots, \langle x_m, y_m \rangle\}$ is :

$$error_S(h) = \frac{1}{m} \sum_{i=1}^{m} \delta(h(x_i) \neq y_i) = \frac{1}{m} \sum_{i=1}^{m} \frac{1 - y_i h(x_i)}{2}$$

and the hypothesis h with the lowest $error_S(h)$ is

$$\arg\max_{h \in H} \frac{1}{m} \sum_{i=1}^{m} y_i h(x_i)$$

Rademacher complexity

Given data sample $S = \{\langle x_1, y_1 \rangle, \ldots, \langle x_m, y_m \rangle\}$
define corresponding set of random labels $\{\sigma_1, \ldots, \sigma_m\}$
where $\sigma_i \in \{-1, 1\}$, $P(\sigma_i = -1) = 0.5 = P(\sigma_i = 1)$.
Note the hypothesis h that best fits these random labels is

$$\arg\max_{h \in H} \frac{1}{m} \sum_{i=1}^{m} \sigma_i h(x_i)$$

Define *empirical Rademacher complexity* $\hat{R}_S(H)$ with respect to S:

$$\hat{R}_S(H) \equiv E_\sigma \left[\max_{h \in H} \frac{1}{m} \sum_{i=1}^{m} \sigma_i h(x_i) \right]$$

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then in the agnostic PAC learning setting, with probability $(1 - \delta)$:

$$error_{true}(h) \leq error_{train}(h) + \hat{R}_{train}(H) + 3\sqrt{\frac{\log(2/\delta)}{m}}$$

Rademacher complexity

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What is $\hat{R}_S(H)$ when:

$H = \{h_1\}$ has only one hypothesis?

H can shatter the training set S?

Rademacher complexity

$$\hat{R}_S(H) \equiv E_\sigma \left[\max_{h \in H} \frac{1}{m} \sum_{i=1}^{m} \sigma_i h(x_i) \right]$$

What is $\hat{R}_S(H)$ when:

$H = \{h_1\}$ has only one hypothesis? $\hat{R}_s(H) = 0$

H can shatter the training set S? $\hat{R}_s(H) = 1$

Empirical Rademacher Complexity

$$\hat{R}_S(H) \equiv E_\sigma \left[\max_{h \in H} \frac{1}{m} \sum_{i=1}^{m} \sigma_i h(x_i) \right]$$

Rademacher complexity:

- applies to real-valued functions (e.g., regression)
- is sensitive to P(X), and particular training set
- can give tighter bounds than VC dimension

Also define full *Rademacher complexity*

$$R_m(H) \equiv E_{S \text{ of size } m}[\hat{R}_S(H)]$$

With probability $\geq (1-\delta)$, $(error_{true} - error_{train}) \leq \epsilon$

(1) for all $h \in H$ such that $error_{train} = 0$,

$$\epsilon = \frac{\ln|H| + \ln(1/\delta)}{m}$$

finite H

(2) for all $h \in H$

Agnostic

$$\epsilon = \sqrt{\frac{\ln|H| + \ln(1/\delta)}{2m}}$$

finite H

(3) for all $h \in H$

Agnostic

$$\epsilon = 8\sqrt{\frac{VC(H)(\ln\frac{m}{VC(H)} + 1) + \ln(8/\delta)}{2m}}$$

infinite H

(4) for all $h \in H$

Agnostic

$$\epsilon = \hat{R}_{train}(H) + 3\sqrt{\frac{\log(2/\delta)}{m}}$$

infinite H